Computational and Experimental Investigation of the Atmospheric Pressure Chemical Vapor Deposition of SiO2 films from TEOS and O2 and Determination of their Microstructural Characteristics and their Corrosion Resistance in Aggressive Aqueous Media.

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Abstract

Chemical vapor deposited SiO2 films from tetraethyl orthosilicate (TEOS) is a key enabling material in numerous applications. Among the several pathways for the CVD of SiO2 films from TEOS, the poorly investigated medium temperature process involving oxygen ensures a compromise between the high temperature TEOS pyrolysis process and the less uniform ozone assisted pathway. It is a promising route for SiO2 coatings on complex-in-shape substrates. In this perspective, we investigate the TEOS+O2 process operating at atmospheric pressure in the temperature range between 350 and 500∘C, for the production of SiOx barrier coatings against aqueous corrosion in fluorine-containing media.

We develop an original apparent kinetic model involving two intermediate species leading to the deposition of SiO2, based on experimentally determined kinetic data and on literature

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information. The numerical simulation of the process reliably reproduces various experimental deposition profiles. The density, strain and stoichiometry of the obtained SiOx films are probed by combining RBS results and FTIR operating under normal and 60◦ incidence angle, especially through the vibrational modes in the 900-1300 cm-1 region with well-resolved TO-LO phonon splitting. Complementary density values obtained by ellipsometry allow estimating the porosity of the films. Their corrosion resistance is investigated by the P-Etch test.

It appears that, with increasing process temperature, the corrosion resistance of the films to P-etch aggressive media increases. This improvement is correlated with LO3 pic evolution that highlights an increase of the SiOx layer density which can be attributed to a decrease of the porosity. Moreover, two types of silica are distinguished. At process temperature lower than 500◦C, SiOxH is observed and at temperature higher than 500◦C, silanol groups disappear. Silica layers with the lowest abrasive P-etch rate expose hydrogen free structure and very low level of porosity.

Keywords: silica film CVD corrosion protection